

Dibenzo-p-dioxin, 1,2,4,7-tetrachloro

Other names:	1,2,4,7-tetrachloro dibenzo-p-dioxin 1,2,4,7-tetrachlorodibenzodioxin
Inchi:	InChI=1S/C12H4Cl4O2/c13-5-1-2-8-9(3-5)18-11-7(15)4-6(14)10(16)12(11)17-8/h1-4H
InchiKey:	SMPHQCMJQUBTFZ-UHFFFAOYSA-N
Formula:	C12H4Cl4O2
SMILES:	Clc1ccc2c(c1)Oc1c(Cl)cc(Cl)c(Cl)c1O2
Mol. weight [g/mol]:	321.97

Physical Properties

Property code	Value	Unit	Source
gf	77.80	kJ/mol	Joback Method
hf	-114.43	kJ/mol	Joback Method
hfus	44.49	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	6.198		Crippen Method
mcvol	182.260	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	2305.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2353.00		NIST Webbook
rinpol	2354.00		NIST Webbook
tb	767.96	K	Joback Method
tc	1035.13	K	Joback Method
tf	551.48	K	Joback Method
vc	0.696	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.63	J/molxK	767.96	Joback Method
cpg	425.28	J/molxK	990.60	Joback Method
cpg	419.14	J/molxK	946.08	Joback Method
cpg	412.71	J/molxK	901.55	Joback Method
cpg	405.89	J/molxK	857.02	Joback Method
cpg	398.57	J/molxK	812.49	Joback Method
cpg	431.25	J/molxK	1035.13	Joback Method
dvisc	0.0004605	Paxs	767.96	Joback Method
dvisc	0.0005188	Paxs	731.88	Joback Method
dvisc	0.0005917	Paxs	695.80	Joback Method
dvisc	0.0006847	Paxs	659.72	Joback Method
dvisc	0.0008058	Paxs	623.64	Joback Method
dvisc	0.0009675	Paxs	587.56	Joback Method
dvisc	0.0011898	Paxs	551.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R37521&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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